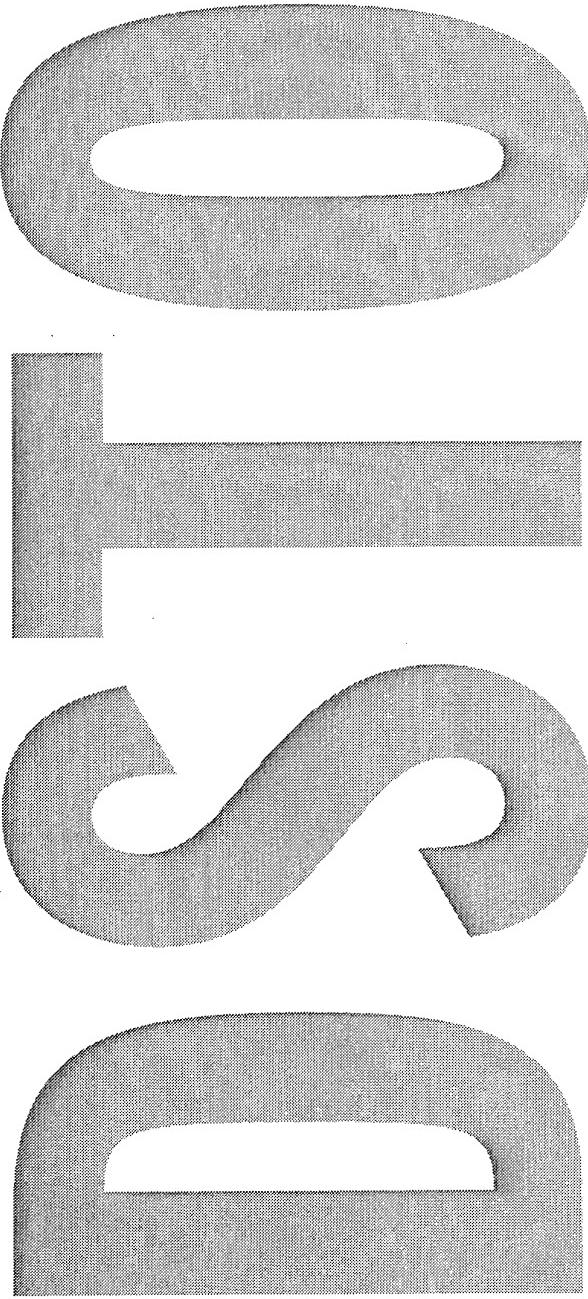




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Fourier Transform Infrared (FTIR) Based Oil Condition Monitoring for Synthetic Turbine Oils

Paul Rawson and Geoff Morris

DSTO-TR-1467

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Paul Rawson and Geoff Morris

Air Vehicles Division
Platforms Sciences Laboratory

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ABSTRACT

To ensure optimum performance of military aircraft engines the chemical and physical condition of their oil must be monitored with time in service. Normal testing methods require a significant cost and time overhead. The ability for one test instrument to monitor the condition of the oil is an essential requirement of modern condition based oil analysis. This paper describes the use of a Fourier Transform Infrared (FTIR) instrument, coupled with the powerful chemometrics based analysis technique to monitor oil acidity, viscosity, load carrying additive, water and antioxidant concentrations from synthetic turbine oils from a series of in-service TF30 engines. The FTIR-Chemometrics based technique was found to offer confident prediction of these oil condition properties and was found to be a suitable technique for oil condition monitoring for the TF30 engine oil system. Further refinement of the technique would be required before introduction into service for use by non-skilled operators.

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Fourier Transform Infrared (FTIR) Based Oil Condition Monitoring for Synthetic Turbine Oils

Executive Summary

The chemical and physical condition of the oil in military aircraft engines must be monitored to ensure optimum performance of the engine and that no damage is done by oil that is too degraded to adequately perform its lubricating role. Routine monitoring requires either expensive laboratory testing or highly skilled analysts. This requirement means that there is a need for a single instrument capable of providing chemical and physical oil condition information. This report describes the use of an automated Fourier Transform Infrared (FTIR) instrument coupled with the statistical based chemometrics analysis technique to determine the chemical and physical condition of synthetic engine oils from the TF30 engine. The FTIR-Chemometrics technique was found to be suitable to determine a range of chemical and physical properties of these oils.

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Paul Rawson graduated with Degree in Applied Science from the University of South Australia in 1986. He joined the AVD Fuel and Lubrication System facility in 1991. The duties in his current position have mainly been involved with research into all aspects of aviation fuel and lubricants for ADF aircraft.

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Geoff Morris came from MOBIL and joined AVD as a contractor to work specifically on TF30 engine oil condition. Geoff also provided scientific support to the AVD investigation into the AVGAS contaminated fuel

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1. Introduction

The ADF has a service on demand policy for aircraft maintenance wherein, for the health of the engine/transmission lubricating systems, only the wear metal content of the lubricating oil is monitored. The oil chemical condition is not taken into consideration for replacement and is expected to remain in a serviceable condition until the engine overhaul period. Oil chemical condition can be a critical factor in early warning of an aircraft propulsion system failure. Periodic monitoring of the chemical condition of the oil is necessary to determine when it has degraded to a point to which it no longer performs its proper function and may also be an indicator for abnormal operation of the engine. Highly degraded oils have the potential to damage aircraft lubricated system components and shorten the life expectancy of the engine or transmission. This situation occurred in Black Hawk main rotor transmissions where the oil had become highly acidic in service, to the degree where it had corroded the magnesium alloy sump in a number of aircraft.

Oil condition monitoring has traditionally been done by performing a range of chemical and physical tests on the oil samples. Molecular analysis of lubricants produces direct information on molecular species of interest, including additive packages, fluid breakdown products and external contamination (1). There are several drawbacks to this practice. These include a relatively large sample being required (up to 100 mL) and several tests which require a chemically trained operator and use of quantities of flammable and hazardous chemicals. Also some of the tests have comparatively poor reproducibility between laboratories.

There has been some development work done by Joint Oil Analysis Program Technical Support Center (JOAP-TSC) to replace some of these tests by the extraction of information from the oil's infrared spectrum. By this means it is possible to determine a number of characteristics such as water content, antiwear additive level, fuel dilution, and the level of ester basestock breakdown. Each of these characteristics is quantified in units of Absorbance/centimetre and not in terms of actual content (2). Two of the most important measurements, oil viscosity and Total Acid Number (TAN) are not determined.

A number of other techniques have been offered as oil condition analysers. However, these analysers usually only monitor one chemical property or determine oil condition by inference. Devices such as the RULER and COBRA have previously been examined for potential as oil condition monitoring tools. The Remaining Useful Life Evaluation Routine (RULER) is a hand-held device using a cyclic voltametric technique to determine oils' antioxidant concentrations. From this antioxidant concentration a remaining useful life value is assigned to the oil.

The Complete Oil Breakdown Rate Analyser (COBRA) is a field portable device using an electrical conductivity technique which is reported to trend closely with TAN (3). These techniques, while useful for specific oil properties, do not measure the whole oil condition. The FTIR offers the potential to determine a number of oil condition parameters in a single

test of the oil, using chemometrics as a data analysis tool. A number of condition property values can be predicted as actual property values rather than inferred condition values.

Chemometrics is the use of mathematical and statistical methods to predict physical and chemical characteristics by indirect methods. Using this analysis it is possible to predict the characteristics of test oils, once a calibration set of samples has been compiled (4).

This report describes a program of work to investigate the potential of FTIR-based oil analysis using chemometric data manipulation to predict a number of oil condition parameters. The oil system chosen was F-111 TF30 engine oil system which uses a synthetic polyol ester based oil conforming to MIL-PRF-23699.

2. Experimental

2.1 Samples

Samples of MIL-PRF-23699 oil were collected from a range of RAAF TF30 engines over a period of four months. A total of ninety samples were tested by traditional laboratory techniques for viscosity at 40°C, Total Acid Number (TAN), antioxidant content, load carrying additive concentration and water. Infrared scans were also performed on each sample. A further 35 samples were collected and used to validate the chemometric modelling procedures.

2.2 Instrumentation and Software

The infrared spectra were collected using a Perkin-Elmer Spectrum 2000 Infrared Spectrometer fitted with a Perkin-Elmer Liquid Autosampler. The final spectra were an average of 16 scans over the range of 4000-450 cm⁻¹ with a resolution of 2 cm⁻¹. The infrared cell was fitted with Zinc Selenide window and had a nominal path length of 0.1 mm. A liquid cell was chosen rather than using Attenuated Total Reflection (ATR) cell because it gave a longer optical path length for the sample. The longer path length results in stronger absorbances for the samples and so gave larger peaks in the weakly absorbing regions. It has the disadvantage that some regions of the spectrum become too strongly absorbing to be useful. These saturated spectral regions are those which are expected to be unchanged due to changes in oil condition and their influence on the predictive model would be insignificant.

The use of a liquid cell also has the advantage of being readily automated, so enabling a large number of samples to be run with minimal operator involvement. The infrared spectra were recorded and processed in absorbance units rather than transmission, because the absorption of the infrared energy by the sample gives a linear response to the concentration of the absorbing material.

The computer software used for the chemometric modelling was Perkin-Elmer Spectrum Quant+.

2.3 Chemometric Modelling

Chemometrics is the use of mathematical and statistical tools to determine by indirect means the properties of a material that would otherwise be difficult or time consuming to measure directly. This approach works as the properties of many materials are governed by their chemical composition and chemical composition can be determined by other means, in this case from infrared spectra. The process to develop a chemometric model involves building the model based on chemical and physical data and infrared spectra of the standards, calibrating the model based on these standards, refining the model to remove anomalous data, and then verifying the model by using it to predict the results for a validation set of samples.

The initial model was developed using analytically measured raw chemical and physical data and the oil's complete infrared spectrum. The physical and chemical data was improved by reanalysing samples that were statistical outliers. Generally, the original statistical outliers were caused by inaccuracies in the physical or chemical test. The modelling process identified these samples as not having the numerical values expected when compared to the infrared spectrum. Also in most cases there were multiple samples from each engine, so comparison with the results of the oil from these samples gave a secondary check on the validity of the results. Another source of outliers were samples where spectral changes were due to non-modelled conditions, such as contamination of the engine oil by incorrect fluids. One instance of this was a number of oils were found to contain the USAF specified MIL-PRF-7808 rather than the RAAF specified MIL-PRF-23699.

As the predictive models were developed from the range of samples available, the distribution of the sample values was not ideal. The ideal set of data would have had values equally distributed across the data range. The uneven distribution of data can be seen from the following breakdown:

Table 1. Oil property data range

Viscosity data	85% [25.4 – 27.6 cSt],	15% [27.6 – 29.4 cSt]
TAN data	86% [0.14 – 0.60 mgKOH/g]	14% [0.60 – 0.97 mgKOH/g]
Antioxidant data	50% [0.10 – 0.30%]	50% [0.30 – 0.75%]

The extreme values for each of the data ranges were dominated by results from oils from a small number of engines (two or three). If the oils from these engines were exhibiting different characteristics to the oil from the other engines, then these results would overly influence the overall results. Some of this effect is shown up in the high leverage shown by some data points. Spectra showing as having high leverage were examined individually to

determine the cause of the high leverage and to see if they could be rejected from the calibration set.

The infrared spectral information for the chemometric model was improved by blanking out areas of high absorption, smoothing the spectra to reduce variation due to noise and adjusting the baseline to correct for changes in the cell transmission. The areas blanked out and so not used in the chemometric model were 3010 to 2820 cm^{-1} (high absorbance due to C-H stretching vibrations), 1790 to 1690 cm^{-1} (high absorbance due the C=O stretching vibrations) and 1495 to 930 cm^{-1} (high absorbance due the C-O stretching vibrations). These areas had absorbances of greater than 1.5 and because of the small amount of energy being transmitted through the sample any small variation due to noise is significant. The smoothing function applied was Savitzky-Golay over 19 points. This smoothed out any peaks due to noise, but also broadened any spectral peaks. The broadening of the spectral peaks does not result in any loss of data, as the peaks in the spectra are relatively wide. Using the derivatives of the spectra for the calculations corrects for any baseline offset or baseline slope in the spectra. Baseline offset can be due to changes in transmission in cell material with age and use. The baseline slope can vary due to solid material (eg fine metal particles and carbonaceous soot in the samples). As the derivative function emphasises narrow features including noise, relative to broad ones, the derivative function is spread over several points. IR spectra which are representative of the differences apparent in the sample are shown in Figure 1. These spectra show subtle differences in the range 3640 to 3120 cm^{-1} , 1670 to 1520 cm^{-1} and 850 to 730 cm^{-1} .

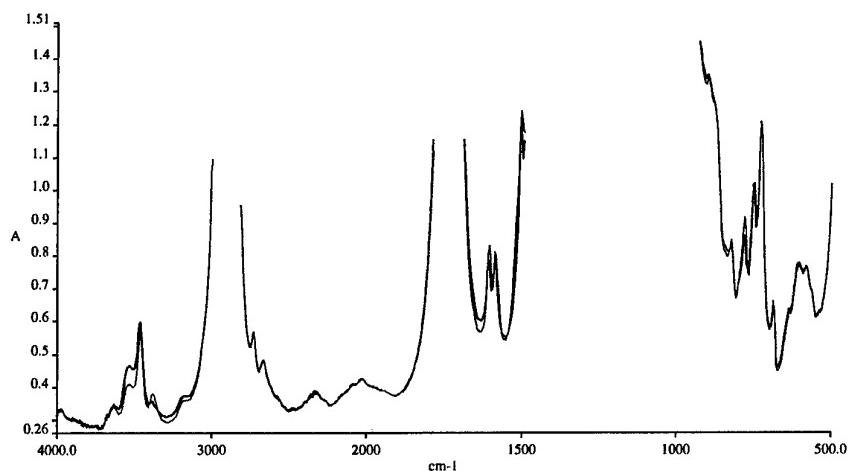


Figure 1. Typical IR Spectra showing the subtle spectral differences between a fresh oil (Blue) and oil from a TF30 engine (Black).

The models for the load-carrying additive and the antioxidant can be further refined by using only spectral regions where the specific compound has significant infrared absorption. These regions can be seen in figures 2 and 3 where overlays of the load-carrying additive and the antioxidant against MIL-PRF-23699 oil are given.

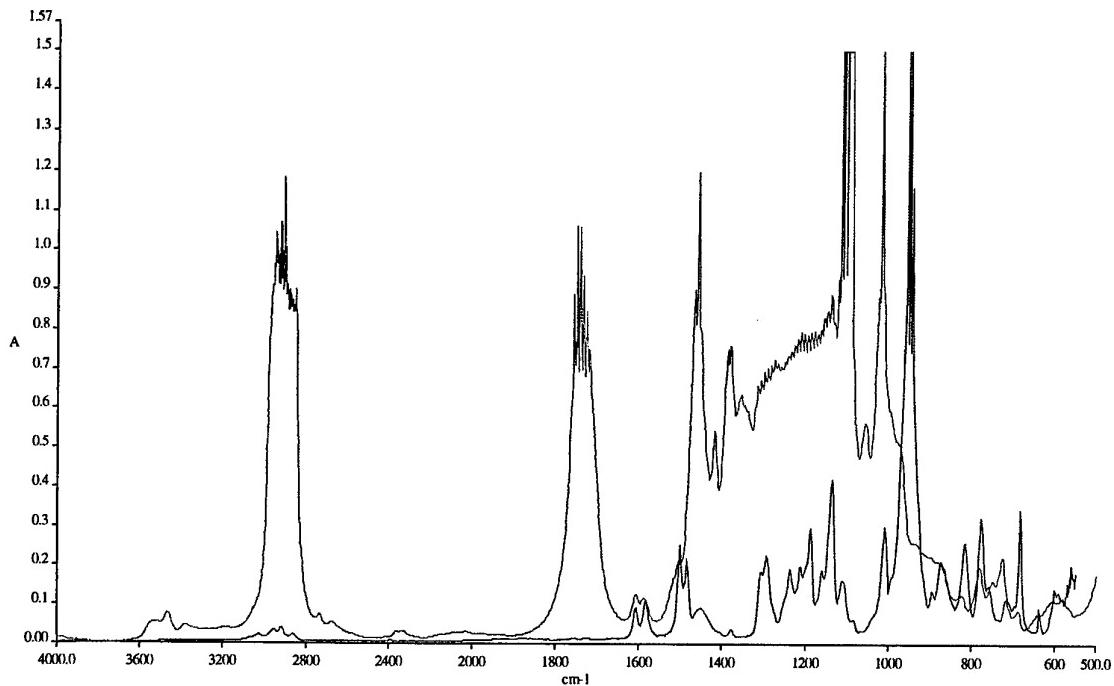


Figure 2. Overlay of MIL-PRF-23699 (green) vs Load Carrying Additive (Tricresyl Phosphate)(red)

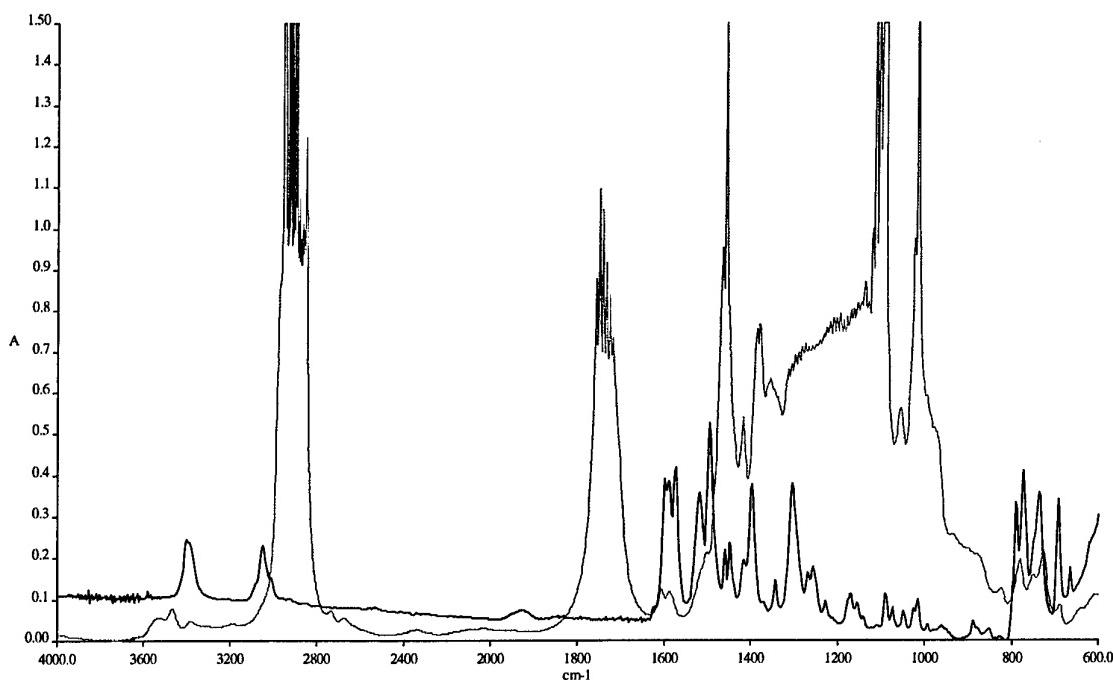


Figure 3. Overlay of MIL-PRF-23699 (green) vs Antioxidant (N-phenyl-1-naphthylamine)(black)

The Perkin-Elmer software offers three multivariate calibration methods Principle Component Regression (PCR), Partial Least Squares (PLS1) and (PLS2). Other multivariate techniques are available, but the modelling was restricted to a choice of these three. The model development was initially conducted using both PCR and PLS. The process of developing the model using PCR involves initially calculating an average spectrum of all the standards, then the average spectrum is compared to each spectrum and a new spectrum, called the factor, describing the differences between the standards and the average is calculated. The amount of the factor in each standard spectrum is calculated and called a score. Next the score for each standard spectrum is multiplied by the factor and this is subtracted from each standard spectrum to produce a residual. This calculated residual is then used to repeat this process. An iterative cycle is carried out until all the significant variations in the standard spectra are accounted for. The calibration using PLS is similar to PCR, but PLS uses oil property concentration data to produce a weighted average spectrum. These mathematical processes are conducted by the computer software program. Software packages such as MATLAB offer chemometric modules allowing the user greater control over the statistical analysis.

The final model chosen used was PLS as this gave the better fit for the data set.

2.4 Model Development

A measure of the "goodness" of the model prediction can be found in the model's Standard Error of Prediction (SEP), that is the magnitude of the error expected when the model is used to predict independent samples.

Optimal SEPs developed from the model are listed in Table 2. and are given at a level to account for 95% of the variance of each oil property.

Table 2. SEP for final PLS predictive model

SEP for Viscosity	SEP for TAN	SEP for Antioxidant	SEP for TCP	SEP for Water
0.24	0.07	0.02	0.06	79

2.4.1 Spread of Principal Components

Examination of the way that the spectrum of each standard is broken down into the major principal components shows that there are groupings based on engine (Figure 4). This grouping implies that each engine is performing slightly differently to the others and so the intricate changes occurring in the oil are slightly different from engine to engine. From examining the chemometric analysis of the engine data it was found that that over 86% of all variance in the model can be attributed to only one principal component and 91.1% by only two principal components. An explanation of principle component analysis is given in appendix D.

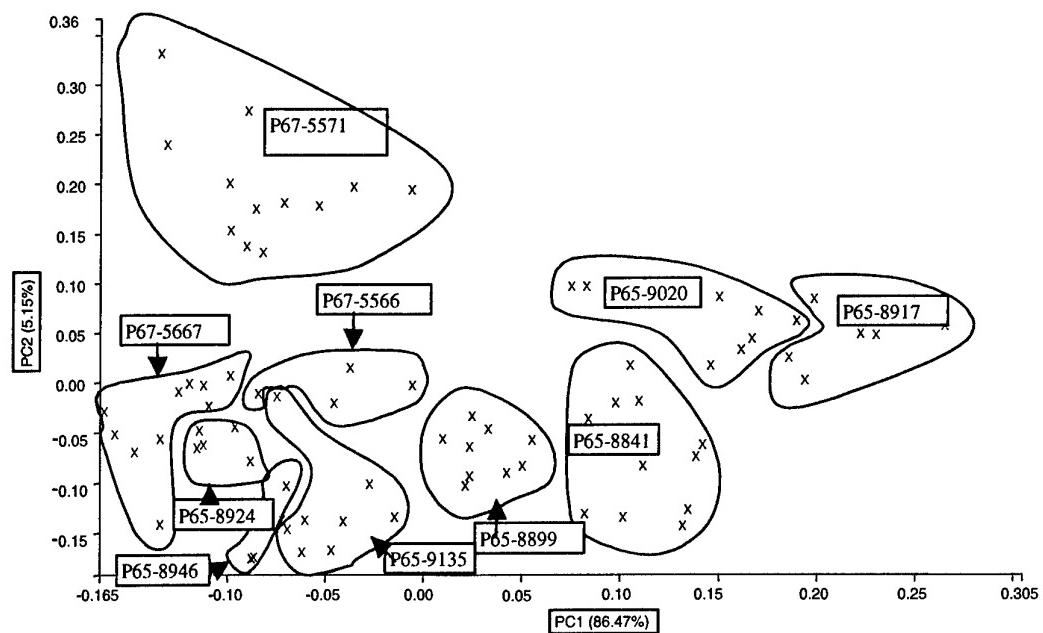


Figure 4 Plot of PC1 versus PC2 for TF30 Engine Oils

2.5 Verification

Once sufficient samples had been obtained to build an effective model, a second batch of samples was accumulated to verify the accuracy of the model. This was done by predicting their property values with the chemometric models and then comparing the predictions against the measured values.

3. Discussion

3.1 Predictive Models

Following optimisation of the data, which was done by rejection of outlier samples, two separate models were developed. One was used to predict the viscosity and the other to predict Total Acid Number (TAN), antioxidant content, load carrying additive concentration and water content. A separate model was developed for fuel dilution using laboratory prepared samples as standards.

3.2 Viscosity Model

The model for predicting viscosity shows good correlation ($R^2 = 0.94$) between the specified and predicted values. When this model is used to predict the values for the validation sample set there is also a good correlation ($R^2=0.96$). The predicted values show a slight bias towards high results of about 0.2 cSt (Figure 5). The results are listed in Appendices A1 and A2.

(Note: The six samples with the lowest viscosities in the chart were found to be mixed with MIL-PRF-7808 oil. This is lower viscosity oil which is also based on a polyol ester. There were no known samples of this type included in the standards used to build the method, but the predicted and measured values are still in agreement.)

The standard error of prediction (SEP) for this model is 0.24 cSt which is worse than the repeatability of the standard ASTM test which is 0.09 cSt. This is considered acceptable, as the normal change in viscosity of the oil over its service life is approximately 5 cSt. Also in using the chemometric models for oil condition monitoring the trends in changes in viscosity are more important than the absolute values and any trends in oil viscosity changes with time are still clear.

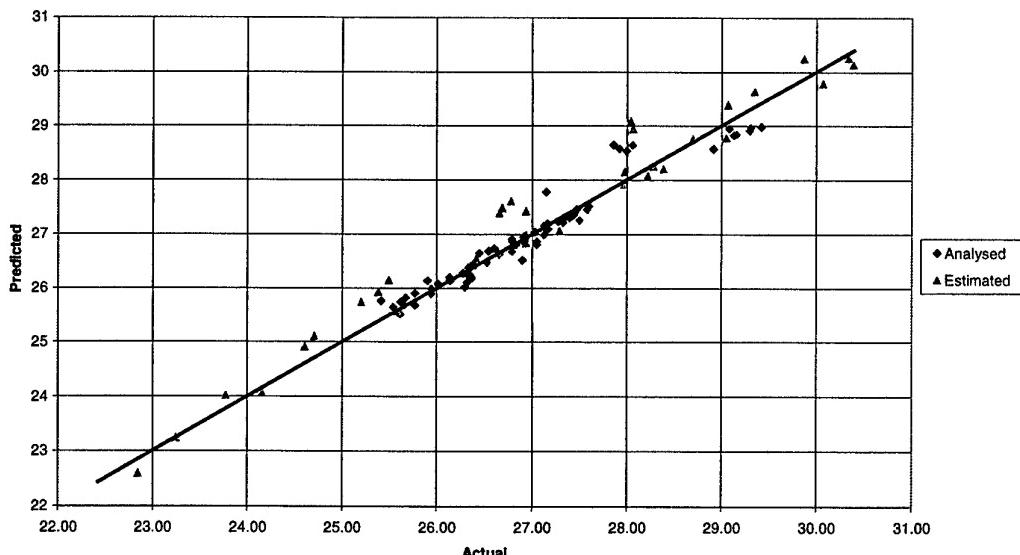


Figure 5. Viscosity Chart

3.3 TAN Model

The model for predicting TAN shows good correlation ($R^2 = 0.92$) between the specified and the estimated values. When it is used to predict the values for the validation samples there was also good correlation ($R^2 = 0.97$) (Figure 6). The results are listed in Appendices A3 and A4.

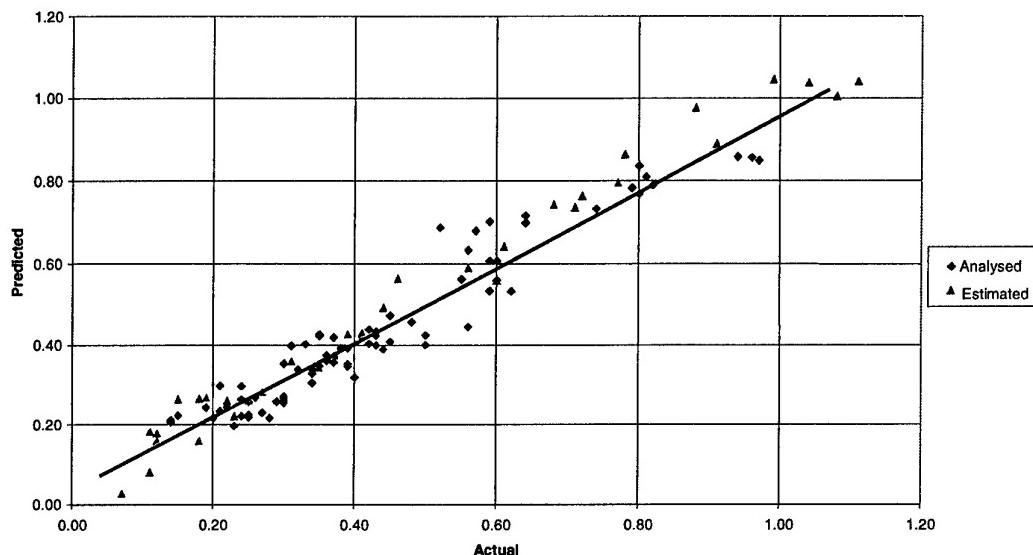


Figure 6. TAN Chart

The standard error of prediction is 0.07 which is equivalent to the repeatability of the standard ASTM chemical test which is approximately 0.06. Both of these errors are much smaller than the variation in TAN over the range of samples tested and the changes that occur over the service life of the oil.

3.4 Antioxidant Content Model

The model for antioxidant content shows very good correlation ($R^2 = 0.99$) between the predicted and measured values. When used to predict the values there is also very good correlation ($R^2 = 0.98$) (Figure 7). The results are listed in Appendices A5 and A6.

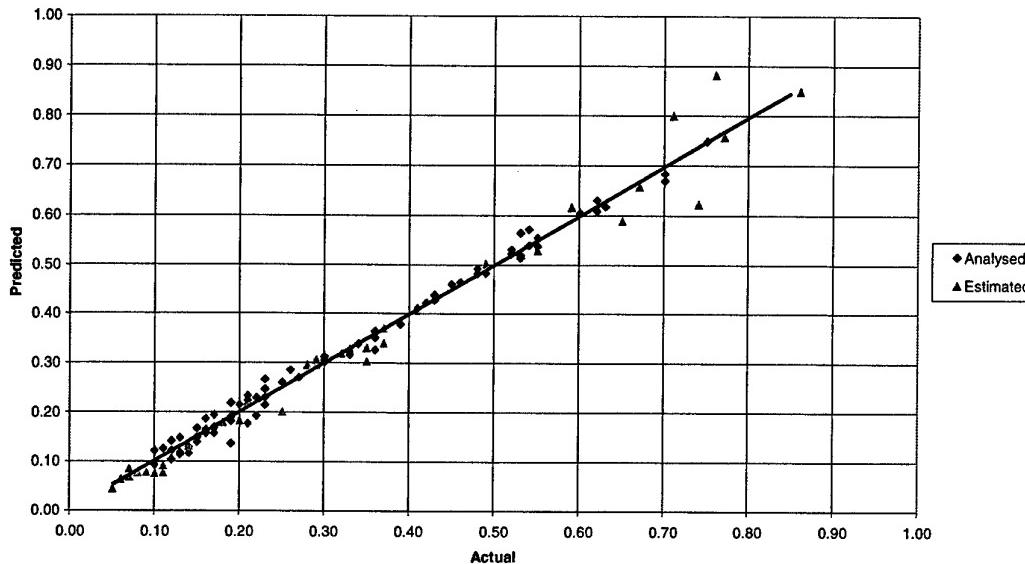


Figure 7. Antioxidant Content Chart

The standard error of prediction for the model is 0.02%. This is small compared to the changes in the antioxidant content over the service life of the oil.

3.5 Load Carrying Additive Concentration Model

The model for the antiwear additive content shows only moderate correlation ($R^2 = 0.68$) between the estimated and the actual results. Much of this poor correlation is most likely due to the accuracy and poor repeatability of the chemical measurement. The correlation of the predicted values also shows only moderate correlation ($R^2 = 0.68$) (Figure 8). Several of the samples were analysed multiple times to reduce the amount of scatter in the results but this was done only on the samples which showed significant variation. The model could possibly have been improved by analysing all the samples multiple times and so eliminate much of the variation. The final results are listed in Appendices A7 and A8.

If the TCP model is separated as was done for the viscosity model, then the R^2 value has been improved to as high as 0.77. It was decided to maintain only two models rather than three due to the requirement of needing to add new data to the models for further oil analysis work, and to expand the calibration set as new engines are added to the database. The use of three predictive models would complicate this model maintenance.

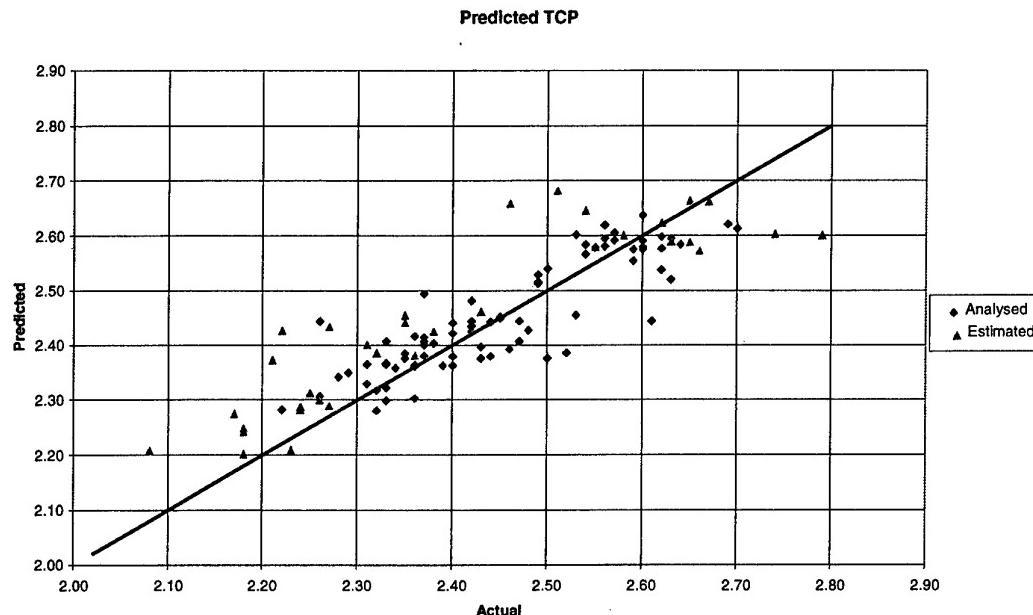


Figure 8. Antiwear Additive Model

Based on the data and multiple measurements for the same sample the repeatability of the chemical test is about 0.12%. The standard error of prediction of the model is 0.06%. Both of these are small compared to the change in the oil over its service life. The prediction model has a slight bias of about 0.05% high when compared to the standards used for the calibration.

3.6 Water Content Model

The model for prediction of the water content showed good correlation between the measured and the estimated values. When the model was used to predict the water content there was a significant bias to giving low values. The reason for this was the hygroscopic nature of the oil. When the model was being developed the majority of the samples had their water contents determined over a short time period regardless of when the samples were taken. The infrared scans were also done over a short time period but at a different time from the water measurements. When the prediction samples were analysed the infrared scans and the water measurements were carried out close together. These differences in the time frame of measurements account for the poor prediction of water content (Figure 9). The results are listed in Appendices A9 and A10.

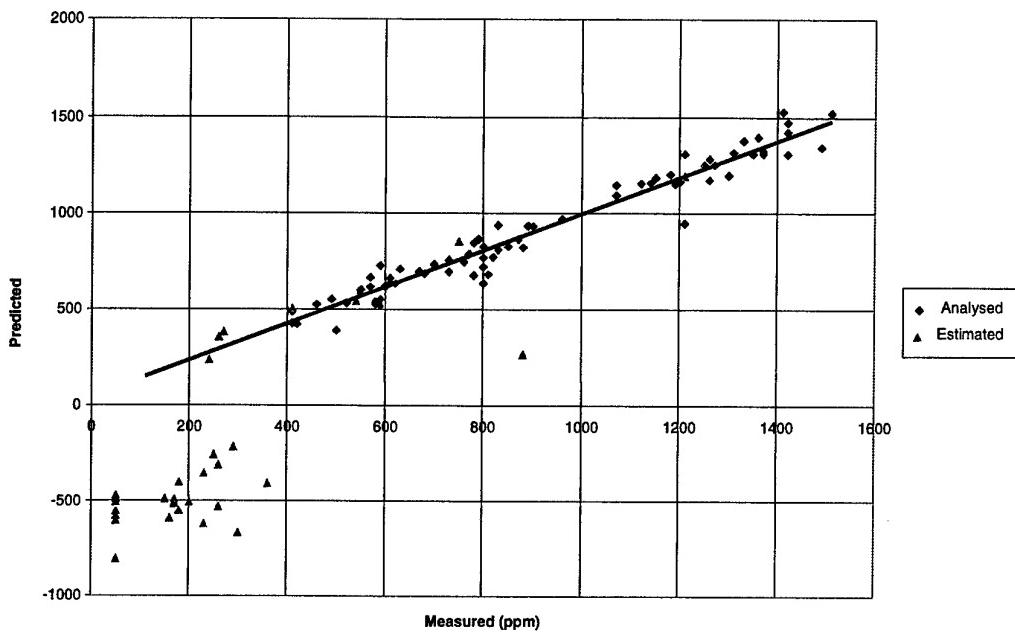


Figure 9. Water Content Model

3.7 Fuel Dilution Model

A small batch of samples was analysed for dilution and contamination with jet fuel. As none was detected in any of the samples tested a model was constructed using laboratory prepared standards. This model was then used to predict the fuel dilution of the engine oil samples. The model displayed good correlation ($R^2 = 0.99$) between the predicted and the known values. However, when it was used to predict the fuel dilution of the engine oil samples the results were found to be engine-dependent, with each engine showing very little change over the range of samples, but with each engine being different from the others. See Appendix A.11.

When a plot of the major PCs is done it shows that the PCs are much more strongly influenced by the oil used to prepare the standards rather than the amount of fuel in the sample (Figure 10). This means that any predictions are more dependent on the nature and condition of the oil than on the degree of fuel contamination. This was an expected result. Experience with laboratory prepared calibration sets has shown that they are not representative of oils degraded in engine service. The chemometric model is not modelling changes in the FTIR spectra wholly due to fuel dilution.

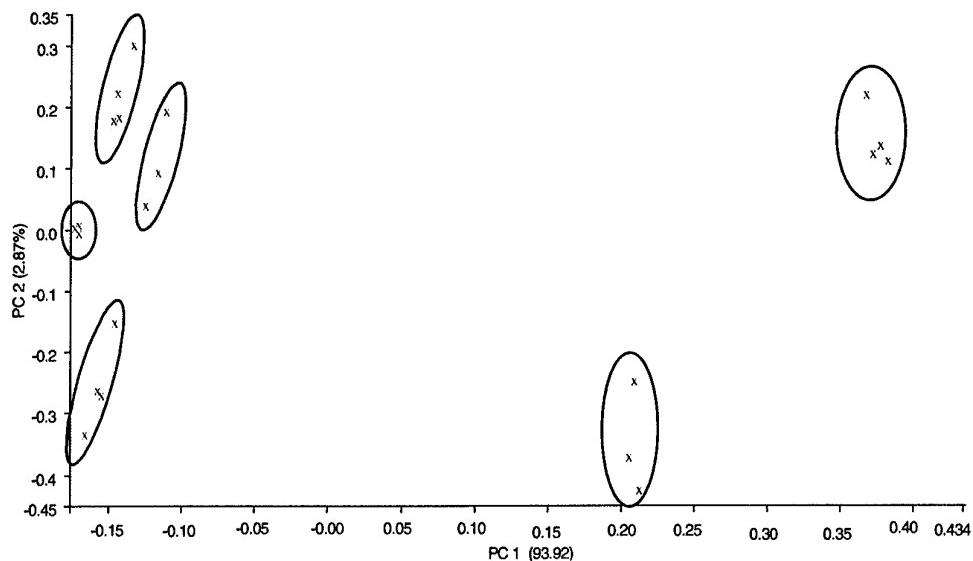


Figure 10. Plot of PC1 versus PC2 for Fuel Dilution Model

3.8 Confidence of Predictions

As part of the calculations for the prediction of results there are two values which give a measure of degree of confidence of the predicted results. These parameters are the Mahalanobis distance (M-distance) ratio and the Residual Ratio. The Mahalanobis distance is a very useful tool for determining the "similarity" of a set of values from an "unknown" sample to a set of values measured from a collection of "known" samples. The M-distance ratio will be less than one for samples within the calibration set. Results greater than one indicate that there are additional features in the sample spectrum that have not been modelled or that the spectral peaks are more intense than the calibration set. The Residual Ratio will be less than three for samples within the calibration range. Values greater than 3 indicate that the sample spectrum contains features not modelled in the calibration set.

The range of M-distance Ratios and Residual Ratios for the different sample groups are shown below.

Model for Viscosity

		M-distance Ratio	Residual Ratio
Calibration Set	Maximum	1.93	5.28
	Minimum	0.108	0.27
Validation Set	Maximum	16.3	111
	Minimum	0.18	1.46

Model for TAN, Antioxidant, Antiwear Additive and Water

		M-distance Ratio	Residual Ratio
Calibration Set	Maximum	1.78	3.98
	Minimum	0.117	0.293
Validation Set	Maximum	35.8	584
	Minimum	0.312	4.87

The high numbers for some of the validation set of samples for both the models for both the M-distance ratio and the Residual Ratio indicate that some of the samples contained spectral information not modelled from the calibration set. This is not unexpected as some of the samples in the validation set were found to contain oil which was not present in the calibration set. Also there are several of the samples in the validation set which have results outside the range of the calibration set for several of the variables. Considering these potential variations and the uncertainty in the results in the validation samples it is slightly surprising that the results for the validation set are so well predicted by the models particularly for viscosity, TAN, Antioxidant Content and Antiwear additive.

Model for Fuel Dilution

		M-distance Ratio	Residual Ratio
Validation Set	Maximum	1.6	37.4
	Minimum	0.10	4.3

The high values for the residual ratios for all the samples in the validation set indicates that the spectra of the samples in the validation set contain features which are not in the spectra of the samples in the calibration set.

3.9 Limitations

There are several areas of limitations for application of these models.

3.9.1 Range of Results

The predicted results are only valid for the range covered in the calibration set. That means that any results that are predicted outside the calibration are to be treated with caution. The ranges of results for the calibration set are listed in Table 2.

Table 2 Range of Values in Calibration Standards

	Viscosity	TAN	Antioxidant	TCP	Water
Range	25.41 - 29.41	0.14 - 0.97	0.10 - 0.75	2.22 - 2.70	410 - 1510

There are several validation samples that have predicted results outside the valid range for each of the characteristics. In most cases (except water content) the predicted results agree with the actual measured results. This may not always be true. To overcome these restrictions and to improve the reliability of the models additional samples covering the extended range of sample results would need to be incorporated into the model calibration set.

3.9.2 Infrared Spectrometer and Cell

If a different infrared spectrometer and/or sample cell is used for the analysis of additional samples a new calibration will need to be done (5). This could be achieved either by rerunning some of the old standards on the new equipment and incorporating them into the model or by running a new set of standards. If the old standards were used there would need to be confidence that the characteristics of the oil had not changed, as there is the possibility for the TAN and water content to change with time.

3.9.3 Age of Model

Chemometric modelling studies have reported changes in accuracy of predictions with time (5). These could be related to changes in the energy output of the infrared source, changes in the spectrometer sensitivity with time or changes in the operating environment of the spectrometer. Any use of the models over a long period of time would need to have a process to compensate for these possible changes. Continual addition of samples to the calibration data set should account for changes in instrument sensitivity. This has been the chosen method for maintaining the models.

3.9.4 Applicability to Other Equipment

An investigation of the applicability of the models to other equipment using MIL-PRF-23699 specification oil was conducted using samples from the main rotor gearboxes of Black Hawk helicopters. When the models were used to predict the values there were considerable differences between the predicted and the actual results for most of the variables (Appendix B). For the viscosity and TAN measurements the predicted values were generally less and in some case much less the actual measured values. For antioxidant content the predictions were close to the measured values. For the TCP content the predicted values were generally higher than the measured values. This disparity between the predicted and measured results would indicate that the chemical processes causing the changes in the oil characteristics are not the same in both applications. In order to predict the values for the oils from the gearboxes a separate model would need to be developed using samples from the gearboxes as the calibration set.

4. Conclusions

Oil condition monitoring for synthetic turbine oils can be performed successfully using FTIR coupled with chemometric modelling. It is possible to accurately determine oil viscosity, TAN, antioxidant concentration, and load carrying additive concentration. The model is not suitable for the prediction of water content but this capability would be easily added with a small amount of extra oil analysis and simple recalibration of the predictive model.

From the models that have been developed it is possible to predict the values of the parameters measured.

Using the model to predict the value for the viscosity, the accuracy of the prediction is worse than the accuracy of the physical test (0.24 versus 0.09 cSt). This deficiency is acceptable as the error associated with the prediction is small when compared to the allowable maximum change in oil viscosity of 5 cSt.

Using the model to predict the value of the TAN, the accuracy of the prediction is equivalent to the chemical test (0.07 versus 0.06 mg KOH/g). By either method the error associated with the result is small compared to the change observed in service.

Using the model to predict the antioxidant content, the accuracy of the prediction is equivalent to the accuracy of the physical test. The error of either test is small compared to the changes that occur as the oil is used.

Using the model to predict the antiwear additive content, the accuracy of the prediction is better than the physical test (0.06 versus 0.12%). In either case the error is small compared to the changes that occur as the oil is used.

The current model is not suitable to predict the water content in the samples. Additional work would need to be done where the water content and the infrared scans are done at the same time to ensure that there are no differences in the oil at the time of the two tests.

The model is not suitable to predict fuel dilution as the model detects the greater variations in the FTIR spectra, which are due to other condition changes in the oil. Spectral changes due to the amount of fuel dilution in the oil are by comparison, very small.

The model is only suitable for prediction of TF30 engine oil condition. Separate models are required if other turbine engine or transmission oils are to be analysed by this technique.

Expansion of the database by continued monitoring of TF30 engine oils will further confirm the validity of the predictive model.

Consideration might also be given to:

- (a) Expanding the model to include a wider range of standards. This will expand the valid range of predictions for the model.
- (b) Examining the applicability of the model to predicting the characteristics of oils from other jet engine systems.
- (c) Investigating the applicability of chemometrics to other aircraft lubricant systems.

5. References

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Appendix A: Test Results

A.1. Measured Viscosity Test Results

Sample Number	Measured Viscosity	Estimated Viscosity
TF30-002	26.65	26.63
TF30-004	26.91	26.85
TF30-005	27.43	27.36
TF30-006	26.89	26.52
TF30-007	27.02	27.04
TF30-009	26.33	26.38
TF30-010	26.52	26.48
TF30-011	26.29	26.01
TF30-013	26.27	26.28
TF30-014	26.44	26.65
TF30-015	26.13	26.13
TF30-018	25.94	25.89
TF30-020	26.14	26.13
TF30-022	26.13	26.20
TF30-024	25.90	26.13
TF30-025	26.82	26.81
TF30-027	26.54	26.69
TF30-029	26.60	26.74
TF30-031	25.61	25.51
TF30-033	25.54	25.65
TF30-034	25.77	25.68
TF30-036	26.90	26.95
TF30-037	27.14	27.10
TF30-040	27.15	27.19
TF30-041	27.16	27.09
TF30-043	27.12	26.99
TF30-045	25.77	25.90
TF30-047	25.65	25.68
TF30-048	25.67	25.82
TF30-049	29.29	28.91
TF30-050	29.07	28.95
TF30-052	29.30	28.96
TF30-053	29.41	28.98
TF30-054	29.15	28.84
TF30-055	29.12	28.83
TF30-057	28.91	28.57

Sample Number	Measured Viscosity	Estimated Viscosity
TF30-060	28.05	28.64
TF30-061	27.91	28.58
TF30-063	27.46	27.46
TF30-067	27.85	28.65
TF30-068	26.92	26.88
TF30-069	26.32	26.24
TF30-070	27.15	27.09
TF30-071	25.94	25.98
TF30-072	26.01	26.09
TF30-074	26.02	26.05
TF30-075	27.57	27.46
TF30-076	26.78	26.68
TF30-077	27.04	26.81
TF30-081	26.36	26.18
TF30-082	26.79	26.87
TF30-083	26.80	26.81
TF30-084	27.99	28.54
TF30-085	27.33	27.30
TF30-087	27.39	27.31
TF30-088	27.32	27.22
TF30-090	27.27	27.23
TF30-091	27.12	27.15
TF30-092	26.31	26.10
TF30-094	27.04	26.87
TF30-096	26.35	26.21
TF30-097	25.41	25.76
TF30-100	26.34	26.25
TF30-102	27.44	27.40
TF30-103	25.62	25.74
TF30-105	27.49	27.26
TF30-107	27.59	27.51
TF30-109	26.38	26.45
TF30-110	26.34	26.37
TF30-111	27.14	27.78
TF30-114	27.41	27.34

A.2. Predicted Viscosity Test Results

Sample Number	Predicted Viscosity	Measured Viscosity
TF30-116	26.84	26.93
TF30-117	26.54	26.41
TF30-118	28.08	28.21
TF30-120	25.57	25.59
TF30-122	27.06	27.28
TF30-123	28.78	29.04
TF30-125	26.66	26.63
TF30-126	27.92	27.96
TF30-127	26.43	26.37
TF30-130	28.95	28.06
TF30-131	28.75	28.69
TF30-132	29.09	28.03
TF30-135	30.13	30.38
TF30-137	29.39	29.06
TF30-139	27.39	26.65
TF30-140	27.48	26.68
TF30-145	27.42	26.93
TF30-146	28.20	28.38

Sample Number	Predicted Viscosity	Measured Viscosity
TF30-147	30.24	29.86
TF30-150	26.98	26.93
TF30-151	27.61	26.77
TF30-152	30.25	30.33
TF30-155	28.25	28.27
TF30-156	29.63	29.34
TF30-157	29.78	30.06
TF30-158	28.15	27.97
TF30-160	25.74	25.20
TF30-161	24.91	24.60
TF30-163	25.93	25.38
TF30-165	25.10	24.70
TF30-167	24.06	24.15
TF30-169	23.24	23.24
TF30-170	22.59	22.84
TF30-172	24.02	23.77
TF30-173	26.15	25.49

A.3. Measured TAN Test Results

Sample Number	Measured TAN	Estimated TAN
TF30-002	0.34	0.33
TF30-004	0.44	0.39
TF30-005	0.45	0.41
TF30-006	0.40	0.32
TF30-007	0.33	0.40
TF30-009	0.62	0.53
TF30-010	0.59	0.53
TF30-011	0.56	0.44
TF30-013	0.45	0.47
TF30-014	0.60	0.56
TF30-015	0.26	0.27
TF30-018	0.30	0.27
TF30-020	0.30	0.27
TF30-022	0.24	0.26
TF30-024	0.24	0.30
TF30-025	0.37	0.36
TF30-026	0.31	0.40
TF30-027	0.36	0.36
TF30-028	0.39	0.35
TF30-029	0.36	0.37
TF30-031	0.14	0.21
TF30-032	0.14	0.21
TF30-033	0.15	0.22
TF30-034	0.23	0.20
TF30-036	0.41	0.42
TF30-037	0.42	0.44
TF30-040	0.48	0.46
TF30-041	0.43	0.43
TF30-043	0.43	0.40
TF30-045	0.20	0.22
TF30-047	0.28	0.22
TF30-048	0.25	0.26
TF30-049	0.97	0.85
TF30-050	0.96	0.86
TF30-052	0.94	0.86
TF30-053	0.81	0.81
TF30-054	0.82	0.79
TF30-055	0.80	0.84
TF30-056	0.79	0.78

Sample Number	Measured TAN	Estimated TAN
TF30-057	0.80	0.77
TF30-058	0.64	0.70
TF30-060	0.59	0.70
TF30-061	0.52	0.69
TF30-063	0.37	0.42
TF30-067	0.74	0.73
TF30-068	0.55	0.56
TF30-069	0.30	0.26
TF30-070	0.60	0.61
TF30-071	0.25	0.22
TF30-072	0.19	0.24
TF30-074	0.25	0.22
TF30-075	0.43	0.42
TF30-076	0.39	0.35
TF30-077	0.34	0.34
TF30-081	0.30	0.25
TF30-082	0.35	0.35
TF30-083	0.32	0.34
TF30-084	0.64	0.72
TF30-085	0.42	0.40
TF30-087	0.50	0.42
TF30-088	0.38	0.39
TF30-090	0.39	0.39
TF30-091	0.59	0.61
TF30-092	0.34	0.30
TF30-094	0.30	0.35
TF30-095	0.21	0.30
TF30-096	0.21	0.23
TF30-097	0.29	0.26
TF30-098	0.37	0.37
TF30-100	0.22	0.24
TF30-102	0.35	0.42
TF30-103	0.27	0.23
TF30-105	0.50	0.40
TF30-107	0.35	0.42
TF30-109	0.25	0.22
TF30-110	0.24	0.22
TF30-111	0.57	0.68
TF30-114	0.56	0.63

A.4. Predicted TAN Test Results

Sample Number	Predicted TAN	Measured TAN
TF30-116	0.36	0.33
TF30-117	0.26	0.24
TF30-118	0.80	0.79
TF30-120	0.22	0.24
TF30-122	0.43	0.43
TF30-123	0.86	0.84
TF30-125	0.28	0.25
TF30-126	0.76	0.75
TF30-127	0.26	0.23
TF30-130	0.74	0.74
TF30-131	0.64	0.64
TF30-132	0.74	0.73
TF30-135	1.04	1.04
TF30-137	0.89	0.88
TF30-139	0.34	0.35
TF30-140	0.49	0.51
TF30-145	0.43	0.42
TF30-146	0.59	0.60

Sample Number	Predicted TAN	Measured TAN
TF30-147	1.04	1.04
TF30-150	0.43	0.44
TF30-151	0.37	0.36
TF30-152	1.05	1.05
TF30-155	0.56	0.58
TF30-156	0.98	0.99
TF30-157	1.00	1.02
TF30-158	0.56	0.57
TF30-160	0.27	0.27
TF30-161	0.18	0.19
TF30-163	0.26	0.26
TF30-165	0.16	0.18
TF30-167	0.18	0.22
TF30-169	0.08	0.11
TF30-170	0.03	0.10
TF30-172	0.16	0.19
TF30-173	0.27	0.25

A.5. Measured Antioxidant Test Results

Sample Number	Measured Antioxidant	Estimated Antioxidant
TF30-002	0.27	0.27
TF30-004	0.23	0.27
TF30-005	0.16	0.16
TF30-006	0.30	0.31
TF30-007	0.21	0.23
TF30-009	0.16	0.16
TF30-010	0.15	0.17
TF30-011	0.16	0.19
TF30-013	0.17	0.17
TF30-014	0.15	0.15
TF30-015	0.53	0.52
TF30-018	0.45	0.46
TF30-020	0.53	0.51
TF30-022	0.52	0.53
TF30-024	0.55	0.54
TF30-025	0.33	0.32
TF30-026	0.39	0.38
TF30-027	0.34	0.34
TF30-028	0.36	0.36
TF30-029	0.36	0.35
TF30-031	0.70	0.68
TF30-032	0.75	0.75
TF30-033	0.70	0.67
TF30-034	0.62	0.63
TF30-036	0.13	0.15
TF30-037	0.12	0.14
TF30-040	0.10	0.12
TF30-041	0.12	0.12
TF30-043	0.16	0.16
TF30-045	0.54	0.57
TF30-047	0.52	0.52
TF30-048	0.62	0.61
TF30-049	0.19	0.22
TF30-050	0.20	0.22
TF30-052	0.21	0.22
TF30-053	0.22	0.23
TF30-054	0.25	0.26
TF30-055	0.23	0.25
TF30-056	0.26	0.29

Sample Number	Measured Antioxidant	Estimated Antioxidant
TF30-057	0.30	0.31
TF30-058	0.16	0.16
TF30-060	0.19	0.14
TF30-061	0.14	0.13
TF30-063	0.13	0.12
TF30-067	0.15	0.14
TF30-068	0.14	0.13
TF30-069	0.49	0.48
TF30-070	0.11	0.13
TF30-071	0.53	0.56
TF30-072	0.55	0.55
TF30-074	0.54	0.54
TF30-075	0.14	0.12
TF30-076	0.33	0.32
TF30-077	0.23	0.23
TF30-081	0.48	0.48
TF30-082	0.33	0.32
TF30-083	0.36	0.33
TF30-084	0.21	0.18
TF30-085	0.19	0.19
TF30-087	0.22	0.19
TF30-088	0.23	0.22
TF30-090	0.17	0.19
TF30-091	0.13	0.11
TF30-092	0.48	0.49
TF30-094	0.21	0.22
TF30-095	0.43	0.43
TF30-096	0.46	0.46
TF30-097	0.63	0.62
TF30-098	0.30	0.30
TF30-100	0.43	0.44
TF30-102	0.19	0.18
TF30-103	0.60	0.60
TF30-105	0.17	0.16
TF30-107	0.17	0.17
TF30-109	0.41	0.41
TF30-110	0.42	0.42
TF30-111	0.12	0.10
TF30-114	0.10	0.09

A.6. Predicted Antioxidant Test Results

Sample Number	Predicted Antioxidant	Measured Antioxidant
TF30-116	0.30	0.35
TF30-117	0.34	0.37
TF30-118	0.08	0.09
TF30-120	0.59	0.65
TF30-122	0.20	0.25
TF30-123	0.08	0.11
TF30-125	0.33	0.35
TF30-126	0.08	0.10
TF30-127	0.37	0.37
TF30-130	0.18	0.18
TF30-131	0.09	0.11
TF30-132	0.18	0.20
TF30-135	0.06	0.06
TF30-137	0.22	0.21
TF30-139	0.32	0.32
TF30-140	0.31	0.29
TF30-145	0.30	0.29
TF30-146	0.13	0.14

Sample Number	Predicted Antioxidant	Measured Antioxidant
TF30-147	0.04	0.05
TF30-150	0.33	0.33
TF30-151	0.30	0.28
TF30-152	0.08	0.08
TF30-155	0.11	0.12
TF30-156	0.07	0.07
TF30-157	0.08	0.07
TF30-158	0.13	0.14
TF30-160	0.62	0.74
TF30-161	0.66	0.67
TF30-163	0.53	0.55
TF30-165	0.62	0.59
TF30-167	0.85	0.86
TF30-169	0.80	0.71
TF30-170	0.88	0.76
TF30-172	0.76	0.77
TF30-173	0.50	0.49

A.7. Measured Antiwear Additive Test Results

Sample Number	Measured Antiwear Additive	Estimated Antiwear Additive
TF30-002	2.62	2.54
TF30-004	2.69	2.62
TF30-005	2.63	2.59
TF30-006	2.76	2.64
TF30-007	2.70	2.61
TF30-009	2.48	2.43
TF30-010	2.40	2.42
TF30-011	2.42	2.44
TF30-013	2.42	2.44
TF30-014	2.37	2.41
TF30-015	2.33	2.36
TF30-018	2.35	2.38
TF30-020	2.40	2.36
TF30-022	2.52	2.39
TF30-024	2.54	2.38
TF30-025	2.47	2.44
TF30-026	2.61	2.44
TF30-027	2.45	2.45
TF30-028	2.53	2.45
TF30-029	2.44	2.44
TF30-031	2.54	2.58
TF30-032	2.62	2.58
TF30-033	2.56	2.58
TF30-034	2.57	2.60
TF30-036	2.37	2.41
TF30-037	2.31	2.36
TF30-040	2.36	2.36
TF30-041	2.36	2.36
TF30-043	2.43	2.40
TF30-045	2.56	2.59
TF30-047	2.64	2.58
TF30-048	2.70	2.58
TF30-049	2.32	2.32
TF30-050	2.22	2.28
TF30-052	2.32	2.28
TF30-053	2.33	2.30
TF30-054	2.26	2.31
TF30-055	2.36	2.30
TF30-056	2.31	2.33

Sample Number	Measured Antiwear Additive	Estimated Antiwear Additive
TF30-057	2.33	2.32
TF30-058	2.47	2.41
TF30-060	2.43	2.38
TF30-061	2.46	2.39
TF30-063	2.56	2.62
TF30-067	2.50	2.38
TF30-068	2.37	2.38
TF30-069	2.44	2.38
TF30-070	2.28	2.34
TF30-071	2.60	2.58
TF30-072	2.59	2.58
TF30-074	2.57	2.59
TF30-075	2.60	2.59
TF30-076	2.36	2.42
TF30-077	2.49	2.52
TF30-081	2.24	2.40
TF30-082	2.26	2.44
TF30-083	2.45	2.45
TF30-084	2.39	2.36
TF30-085	2.50	2.54
TF30-087	2.63	2.52
TF30-088	2.49	2.53
TF30-090	2.60	2.57
TF30-091	2.34	2.36
TF30-092	2.40	2.38
TF30-094	2.37	2.49
TF30-095	2.33	2.37
TF30-096	2.33	2.41
TF30-097	2.59	2.55
TF30-098	2.40	2.44
TF30-100	2.37	2.40
TF30-102	2.49	2.52
TF30-103	2.54	2.57
TF30-105	2.42	2.48
TF30-107	2.49	2.51
TF30-109	2.62	2.60
TF30-110	2.53	2.60
TF30-111	2.29	2.35
TF30-114	2.34	2.36

A.8. Predicted Antiwear Additive Test Results

Sample Number	Predicted Antiwear Additive	Measured Antiwear Additive
TF30-116	2.43	2.42
TF30-117	2.60	2.58
TF30-118	2.30	2.27
TF30-120	2.57	2.58
TF30-122	2.46	2.42
TF30-123	2.24	2.20
TF30-125	2.59	2.58
TF30-126	2.31	2.29
TF30-127	2.58	2.60
TF30-130	2.39	2.32
TF30-131	2.27	2.13
TF30-132	2.43	2.35
TF30-135	2.20	2.07
TF30-137	2.25	2.13
TF30-139	2.66	2.56
TF30-140	2.43	2.37
TF30-145	2.45	2.36
TF30-146	2.29	2.13

Sample Number	Predicted Antiwear Additive	Measured Antiwear Additive
TF30-147	2.29	2.15
TF30-150	2.42	2.32
TF30-151	2.65	2.57
TF30-152	2.21	2.08
TF30-155	2.37	2.20
TF30-156	2.28	2.16
TF30-157	2.21	2.07
TF30-158	2.38	2.26
TF30-160	2.62	2.58
TF30-161	2.59	2.50
TF30-163	2.66	2.60
TF30-165	2.66	2.52
TF30-167	2.50	2.38
TF30-169	2.40	2.25
TF30-170	2.44	2.23
TF30-172	2.60	2.51
TF30-173	2.68	2.65

A.9. Measured Water Test Results

Sample Number	Measured Water Content	Estimated Water Content
TF30-002	N M	1080
TF30-004	1140	1159
TF30-005	600	616
TF30-006	830	810
TF30-007	1190	1150
TF30-009	1180	1203
TF30-010	1150	1184
TF30-011	830	937
TF30-013	850	826
TF30-014	1200	1165
TF30-015	870	864
TF30-018	1410	1525
TF30-020	800	826
TF30-022	730	757
TF30-024	1420	1307
TF30-025	800	771
TF30-026	1510	1521
TF30-027	1070	1092
TF30-028	N M	1019
TF30-029	1070	1146
TF30-031	960	969
TF30-032	N M	1025
TF30-033	890	933
TF30-034	620	635
TF30-036	1330	1377
TF30-037	1270	1251
TF30-040	1310	1317
TF30-041	1260	1283
TF30-043	900	932
TF30-045	880	822
TF30-047	1420	1473
TF30-048	1350	1309
TF30-049	1360	1397
TF30-050	1490	1343
TF30-052	1370	1311
TF30-053	590	726
TF30-054	770	789
TF30-055	1370	1323
TF30-056	N M	1207

Sample Number	Measured Water Content	Estimated Water Content
TF30-057	780	844
TF30-058	N M	1562
TF30-060	790	865
TF30-061	N M	941
TF30-063	820	773
TF30-067	1120	1155
TF30-068	780	676
TF30-069	610	637
TF30-070	630	709
TF30-071	610	662
TF30-072	790	864
TF30-074	760	746
TF30-075	670	697
TF30-076	800	720
TF30-077	570	665
TF30-081	570	616
TF30-082	800	637
TF30-083	520	531
TF30-084	1250	1252
TF30-085	590	552
TF30-087	600	619
TF30-088	580	536
TF30-090	550	601
TF30-091	810	682
TF30-092	1210	1308
TF30-094	700	734
TF30-095	1300	1196
TF30-096	410	485
TF30-097	1420	1423
TF30-098	1210	947
TF30-100	730	696
TF30-102	580	527
TF30-103	1260	1173
TF30-105	490	552
TF30-107	460	523
TF30-109	500	390
TF30-110	410	426
TF30-111	420	420
TF30-114	680	685

A.10. Predicted Water Test Results

Sample Number	Predicted Water Content	Measured Water Content
TF30-116	355	260
TF30-117	530	590
TF30-118	500	410
TF30-120	1190	1210
TF30-122	850	750
TF30-123	240	240
TF30-125	380	270
TF30-126	540	540
TF30-127	600	550
TF30-130	-220	290
TF30-131	-600	50
TF30-132	-310	260
TF30-135	-560	50
TF30-137	-620	230
TF30-139	-410	360
TF30-140	260	880
TF30-145	-490	50
TF30-146	-490	170

Sample Number	Predicted Water Content	Measured Water Content
TF30-147	-510	170
TF30-150	-400	180
TF30-151	-520	170
TF30-152	-590	160
TF30-155	-470	50
TF30-156	-260	250
TF30-157	-490	150
TF30-158	-360	230
TF30-160	-510	170
TF30-161	-510	50
TF30-163	-530	260
TF30-165	-670	300
TF30-167	-500	170
TF30-169	-810	50
TF30-170	-550	180
TF30-172	-510	200
TF30-173	-580	50

A.11. Predicted Fuel Dilution Results by Engine

Sample Number	Predicted Fuel Dilution
TF30-024	1.8
TF30-022	1.7
TF30-020	2.2
TF30-018	2.4
TF30-015	2.2
TF30-069	1.9
TF30-092	2.4
TF30-081	1.7
TF30-096	1.6
TF30-100	1.8
TF30-095	2.3

Sample Number	Predicted Fuel Dilution
TF30-028	1.2
TF30-026	1.2
TF30-029	1.1
TF30-027	1.2
TF30-025	1.1
TF30-076	2.2
TF30-083	0.7
TF30-082	0.9
TF30-098	0.9
TF30-116	1.3

Sample Number	Predicted Fuel Dilution
TF30-032	1.4
TF30-031	1.5
TF30-033	1.3
TF30-034	1.1
TF30-097	1.6
TF30-103	1.6
TF30-120	1.7

Sample Number	Predicted Fuel Dilution
TF30-058	1.3
TF30-061	1.3
TF30-060	1.1
TF30-067	1.3
TF30-084	1.0

Sample Number	Predicted Fuel Dilution
TF30-036	1.4
TF30-043	1.2
TF30-041	1.5
TF30-040	1.3
TF30-037	1.3

Sample Number	Predicted Fuel Dilution
TF30-048	0.7
TF30-045	0.3
TF30-047	0.6
TF30-071	0.4
TF30-072	0.4
TF30-074	0.3
TF30-110	0.0
TF30-109	-0.1
TF30-127	0.6
TF30-117	0.4
TF30-125	0.4

Sample Number	Predicted Fuel Dilution
TF30-057	1.7
TF30-056	1.8
TF30-055	1.7
TF30-054	1.5
TF30-053	1.5
TF30-052	1.5
TF30-050	1.7
TF30-049	1.4

Sample Number	Predicted Fuel Dilution
TF30-002	0.0
TF30-077	0.8
TF30-094	1.0
TF30-105	0.8
TF30-122	1.0

Sample Number	Predicted Fuel Dilution
TF30-006	1.5
TF30-004	1.5
TF30-007	1.5
TF30-005	1.4
TF30-063	0.5
TF30-075	1.2
TF30-090	1.2
TF30-085	1.4
TF30-087	1.4
TF30-088	1.3
TF30-102	1.3
TF30-107	1.1

Sample Number	Predicted Fuel Dilution
TF30-011	3.0
TF30-013	2.9
TF30-009	2.9
TF30-010	2.7
TF30-014	2.8
TF30-068	2.5
TF30-070	2.9
TF30-091	3.0
TF30-114	2.5
TF30-111	2.5
TF30-126	3.1
TF30-118	3.1
TF30-123	3.1

Appendix B: Other Equipment Predictions

B.1. Predicted Viscosity Results

Sample Number	Predicted Viscosity	Measured Viscosity
105-0858	18.24	24.19
105-1068	24.16	24.44
105-1168	24.01	24.63
105-1233	24.20	24.50
105-1333	24.94	24.52
105-1426	25.10	24.59
106-1180	17.61	23.75
106-1365	24.07	24.66
106-1552	24.29	24.73
106-1696	24.68	24.39
106-1796	24.26	24.30
106-1895	24.45	24.09
109-0582	24.15	24.36
109-0675	24.54	24.37
109-0866	24.44	24.54
109-1021	24.02	24.84
109-1116	24.06	24.72
109-1315	21.27	19.11
109-1620	24.22	23.92
114-0779	20.87	24.52
114-0878	20.79	24.01
114-1174	21.09	22.85
114-1272	21.25	23.07

Sample Number	Predicted Viscosity	Measured Viscosity
114-1572	22.08	22.75
114-1670	23.95	23.69
114-1763	23.38	22.95
114-1876	23.28	22.76
201-0364	7.99	23.90
201-0599	9.81	23.97
201-0691	11.06	24.04
201-0890	12.36	23.99
203-0010	22.17	24.44
203-0677	19.66	24.34
203-0769	20.12	24.40
203-0863	20.21	24.32
203-1114	20.28	24.65
203-1273	22.54	24.31
203-1672	24.81	24.66
212-0583	21.55	24.45
212-0689	21.78	24.49
212-0973	22.66	24.67
212-1094	22.45	24.26
212-1294	22.41	23.37
222-0387	21.69	24.46
222-0485	22.01	24.49

B.2. Predicted TAN Results

Sample Number	Predicted TAN	Measured TAN
105-0858	0.12	7.71
105-1068	0.26	0.87
105-1168	0.15	0.61
105-1233	0.24	0.78
105-1333	0.33	0.69
105-1426	0.32	0.64
106-1180	0.28	15.63
106-1365	0.29	1.90
106-1552	0.28	1.19
106-1696	0.26	0.50
106-1796	0.24	0.21
106-1895	0.24	1.10
109-0582	0.24	0.75
109-0675	0.25	1.28
109-0866	0.22	1.07
109-1021	0.17	1.38
109-1116	0.16	0.35
109-1315	-0.02	0.35
109-1620	0.21	0.20
114-0779	-0.04	2.49
114-0878	-0.04	2.15
114-1174	-0.03	1.58
114-1272	-0.03	1.47

Sample Number	Predicted TAN	Measured TAN
114-1572	0.03	1.31
114-1670	0.16	0.47
114-1763	0.12	2.19
114-1876	0.10	1.66
201-0364	-0.28	2.79
201-0599	-0.28	2.16
201-0691	-0.24	1.63
201-0890	-0.12	1.85
203-0010	-0.01	0.29
203-0677	-0.07	2.84
203-0769	-0.03	5.36
203-0863	-0.03	1.96
203-1114	-0.14	1.45
203-1273	0.03	0.47
203-1672	0.29	1.12
212-0583	0.02	2.44
212-0689	0.01	1.53
212-0973	0.07	1.15
212-1094	0.04	2.48
212-1294	0.05	1.08
222-0387	0.11	2.18
222-0485	0.13	2.07

B.3. Predicted Antioxidant Results

Sample Number	Predicted Antioxidant	Measured Antioxidant
105-0858	0.88	0.81
105-1068	0.92	0.91
105-1168	0.91	0.90
105-1233	0.88	0.87
105-1333	0.87	0.91
105-1426	0.86	0.90
106-1180	0.84	0.70
106-1365	0.86	0.79
106-1552	0.87	0.82
106-1696	0.86	0.90
106-1796	0.89	0.94
106-1895	0.89	0.95
109-0582	0.94	0.97
109-0675	0.95	0.95
109-0866	0.91	0.91
109-1021	0.88	0.89
109-1116	0.86	0.87
109-1315	0.74	0.70
109-1620	0.82	0.86
114-0779	0.72	0.69
114-0878	0.71	0.67
114-1174	0.68	0.65
114-1272	0.66	0.63

Sample Number	Predicted Antioxidant	Measured Antioxidant
114-1572	0.67	0.64
114-1670	0.83	0.87
114-1763	0.76	0.79
114-1876	0.74	N M
201-0364	1.03	N M
201-0599	1.00	0.79
201-0691	0.95	0.76
201-0890	0.92	N M
203-0010	0.77	0.81
203-0677	0.77	0.75
203-0769	0.76	0.73
203-0863	0.76	0.72
203-1114	0.74	0.69
203-1273	0.77	0.79
203-1672	0.90	0.98
212-0583	0.79	0.77
212-0689	0.80	0.79
212-0973	0.80	0.79
212-1094	0.78	0.77
212-1294	0.75	N M
222-0387	0.74	0.75
222-0485	0.72	0.71

B.4. Predicted Antiwear Additive Results

Sample Number	Predicted TCP	Measured TCP
105-0858	2.44	1.90
105-1068	2.34	2.21
105-1168	2.32	2.08
105-1233	2.38	2.29
105-1333	2.59	2.61
105-1426	2.60	2.47
106-1180	2.46	1.95
106-1365	2.35	2.14
106-1552	2.35	2.08
106-1696	2.48	2.40
106-1796	2.51	2.50
106-1895	2.47	2.67
109-0582	2.19	2.27
109-0675	2.19	2.09
109-0866	2.22	2.17
109-1021	2.29	2.19
109-1116	2.32	2.07
109-1315	2.07	1.78
109-1620	2.54	2.42
114-0779	2.29	1.76
114-0878	2.27	1.71
114-1174	2.27	1.82
114-1272	2.31	1.98

Sample Number	Predicted TCP	Measured TCP
114-1572	2.35	1.86
114-1670	2.53	2.60
114-1763	2.53	2.34
114-1876	2.50	N M
201-0364	2.66	N M
201-0599	2.59	2.17
201-0691	2.62	2.27
201-0890	2.63	N M
203-0010	2.43	2.32
203-0677	2.29	1.66
203-0769	2.29	1.67
203-0863	2.30	1.66
203-1114	2.32	1.82
203-1273	2.48	2.24
203-1672	2.53	2.57
212-0583	2.24	1.73
212-0689	2.25	1.71
212-0973	2.28	1.92
212-1094	2.26	1.78
212-1294	2.28	N M
222-0387	2.17	1.69
222-0485	2.17	1.74

Appendix C: Summary of Models

These summaries are specific for the Perkin-Elmer Quant+ software and describe the FTIR and chemometric program setup for each successful model.

C.1. Model for Viscosity

Method Summary: tf30v

Method:

Name: tf30v

Ident: PE IR SubTech Method BINARY QUANT+ 4.00

Version: 1

ID: 388

Analyst: GAM

Title:

Description: Analysis of Viscosity in Mobil Jet Oil II from TF30
engines

Created: 05/22/2000 13:15:23

Last modified: 06/22/2000 11:41:09

Secured: No

No. of properties: 1

No. of standards: 78

Calibrated: Yes

Calculation Parameters:

Algorithm: PLS2

Range: 4000 to 500 cm⁻¹

Interval: 1 cm⁻¹

Analysis Type: Absorbance

Scaling (Spectra): Mean

Scaling (Property): Mean

Smooth: Yes

Smooth width: 25

Baseline correction: Derivative

Order: 2

Width: 9

Normalization: Norm. Factor

Ordinate threshold:

Upper threshold: 1.5 A

Lower threshold: None

Number of factors:

Minimum: 1

Maximum: 100
Blank regions: 3010.00 to 2820.00 1790.00 to 1690.00 cm-1
1495.00 to 930.00 cm-1

Property Values:

Standards:	Norm. Factor	Viscosity
tf30-002	0.1126	26.6500 cSt
tf30-004	0.1126	26.9100 cSt
tf30-005	0.1126	27.4300 cSt
tf30-006	0.1126	26.8900 cSt
tf30-007	0.1126	27.0200 cSt
tf30-009	0.1126	26.3300 cSt
tf30-010	0.1126	26.5200 cSt
tf30-011	0.1126	26.2900 cSt
tf30-013	0.1126	26.2700 cSt
tf30-014	0.1126	26.4400 cSt
tf30-015	0.1126	26.1300 cSt
tf30-018	0.1126	25.9400 cSt
tf30-020	0.1126	26.1400 cSt
tf30-022	0.1126	26.1300 cSt
tf30-024	0.1126	25.9000 cSt
tf30-025	0.1126	26.8200 cSt
tf30-026	0.1126	Unknown cSt
tf30-027	0.1126	26.5400 cSt
tf30-028	0.1126	Unknown cSt
tf30-029	0.1126	26.6000 cSt
tf30-031	0.1126	25.6100 cSt
tf30-032	0.1126	Unknown cSt
tf30-033	0.1126	25.5400 cSt
tf30-034	0.1126	25.7700 cSt
tf30-036	0.1126	26.9000 cSt
tf30-037	0.1126	27.1400 cSt
tf30-040	0.1126	27.1500 cSt
tf30-041	0.1126	27.1600 cSt
tf30-043	0.1126	27.1200 cSt
tf30-045	0.1126	25.7700 cSt
tf30-047	0.1126	25.6500 cSt
tf30-048	0.1126	25.6700 cSt
tf30-049	0.1126	29.2900 cSt
tf30-050	0.1126	29.0700 cSt
tf30-052	0.1126	29.3000 cSt
tf30-053	0.1126	29.4100 cSt
tf30-054	0.1126	29.1500 cSt
tf30-055	0.1126	29.1200 cSt

tf30-056	0.1126	Unknown cSt
tf30-057	0.1126	28.9100 cSt
tf30-058	0.1126	Unknown cSt
tf30-060	0.1126	28.0500 cSt
tf30-061	0.1126	27.9100 cSt
tf30-063	0.1126	27.4600 cSt
tf30-067	0.1126	27.8500 cSt
tf30-068	0.1126	26.9200 cSt
tf30-069	0.1126	26.3200 cSt
tf30-070	0.1126	27.1500 cSt
tf30-071	0.1126	25.9400 cSt
tf30-072	0.1126	26.0100 cSt
tf30-074	0.1126	26.0200 cSt
tf30-075	0.1126	27.5700 cSt
tf30-076	0.1126	26.7800 cSt
tf30-077	0.1126	27.0400 cSt
tf30-081	0.1126	26.3600 cSt
tf30-082	0.1126	26.7900 cSt
tf30-083	0.1126	26.8000 cSt
tf30-084	0.1126	27.9900 cSt
tf30-085	0.1126	27.3300 cSt
tf30-087	0.1126	27.3900 cSt
tf30-088	0.1126	27.3200 cSt
tf30-090	0.1126	27.2700 cSt
tf30-091	0.1126	27.1200 cSt
tf30-092	0.1126	26.3100 cSt
tf30-094	0.1126	27.0400 cSt
tf30-095	0.1126	Unknown cSt
tf30-096	0.1126	26.3500 cSt
tf30-097	0.1126	25.4100 cSt
tf30-098	0.1126	26.7800 cSt
tf30-100	0.1126	26.3400 cSt
tf30-102	0.1126	27.4400 cSt
tf30-103	0.1126	25.6200 cSt
tf30-105	0.1126	27.4900 cSt
tf30-107	0.1126	27.5900 cSt
tf30-109	0.1126	26.3800 cSt
tf30-110	0.1126	26.3400 cSt
tf30-111	0.1126	27.1400 cSt
tf30-114	0.1126	27.4100 cSt

C.2. Model for TAN, Antioxidant, TCP and Water

Method Summary: tf30t

Method:

Name: tf30t
Ident: PE IR SubTech Method BINARY QUANT+ 4.00
Version: 2
ID: 3144
Analyst: gam
Title:
Description: Analysis of TAN, Antioxidant, TCP and Water in Mobil Jet
Oil II from TF30 engines
Created: 05/11/2000 09:37:56
Last modified: 07/12/2000 12:25:17
Secured: No
No. of properties: 4
No. of standards: 78
Calibrated: Yes

Calculation Parameters:

Algorithm: PLS2
Range: 4000 to 500 cm⁻¹
Interval: 1 cm⁻¹
Analysis Type: Absorbance
Scaling (Spectra): Mean
Scaling (Property): Mean
Smooth: Yes
Smooth width: 19
Baseline correction: Derivative
Order: 2
Width: 9
Normalization: Norm. Factor
Ordinate threshold:
Upper threshold: 1.5 A
Lower threshold: None
Number of factors:
Minimum: 1
Maximum: 100
Blank regions: 3010.00 to 2820.00 1790.00 to 1690.00 cm⁻¹
1495.00 to 930.00 cm⁻¹

Property Values:

Standards:	Norm. Factor	TAN	Antioxidant
tf30-002	0.1126	0.3400	0.2700 %
tf30-004	0.1126	0.4400	0.2300 %
tf30-005	0.1126	0.4500	0.1600 %
tf30-006	0.1126	0.4000	0.3000 %
tf30-007	0.1126	0.3300	0.2100 %
tf30-009	0.1126	0.6200	0.1600 %
tf30-010	0.1126	0.5900	0.1500 %
tf30-011	0.1126	0.5600	0.1600 %
tf30-013	0.1126	0.4500	0.1700 %
tf30-014	0.1126	0.6000	0.1500 %
tf30-015	0.1126	0.2600	0.5300 %
tf30-018	0.1126	0.3000	0.4500 %
tf30-020	0.1126	0.3000	0.5300 %
tf30-022	0.1126	0.2400	0.5200 %
tf30-024	0.1126	0.2400	0.5500 %
tf30-025	0.1126	0.3700	0.3300 %
tf30-026	0.1126	0.3100	0.3900 %
tf30-027	0.1126	0.3600	0.3400 %
tf30-028	0.1126	0.3900	0.3600 %
tf30-029	0.1126	0.3600	0.3600 %
tf30-031	0.1126	0.1400	0.7000 %
tf30-032	0.1126	0.1400	0.7500 %
tf30-033	0.1126	0.1500	0.7000 %
tf30-034	0.1126	0.2300	0.6200 %
tf30-036	0.1126	0.4100	0.1300 %
tf30-037	0.1126	0.4200	0.1200 %
tf30-040	0.1126	0.4800	0.1000 %
tf30-041	0.1126	0.4300	0.1200 %
tf30-043	0.1126	0.4300	0.1600 %
tf30-045	0.1126	0.2000	0.5400 %
tf30-047	0.1126	0.2800	0.5200 %
tf30-048	0.1126	0.2500	0.6200 %
tf30-049	0.1126	0.9700	0.1900 %
tf30-050	0.1126	0.9600	0.2000 %
tf30-052	0.1126	0.9400	0.2100 %
tf30-053	0.1126	0.8100	0.2200 %
tf30-054	0.1126	0.8200	0.2500 %
tf30-055	0.1126	0.8000	0.2300 %
tf30-056	0.1126	0.7900	0.2600 %
tf30-057	0.1126	0.8000	0.3000 %
tf30-058	0.1126	0.6400	0.1600 %
tf30-060	0.1126	0.5900	0.1900 %
tf30-061	0.1126	0.5200	0.1400 %
tf30-063	0.1126	0.3700	0.1300 %

tf30-067	0.1126	0.7400	0.1500 %
tf30-068	0.1126	0.5500	0.1400 %
tf30-069	0.1126	0.3000	0.4900 %
tf30-070	0.1126	0.6000	0.1100 %
tf30-071	0.1126	0.2500	0.5300 %
tf30-072	0.1126	0.1900	0.5500 %
tf30-074	0.1126	0.2500	0.5400 %
tf30-075	0.1126	0.4300	0.1400 %
tf30-076	0.1126	0.3900	0.3300 %
tf30-077	0.1126	0.3400	0.2300 %
tf30-081	0.1126	0.3000	0.4800 %
tf30-082	0.1126	0.3500	0.3300 %
tf30-083	0.1126	0.3200	0.3600 %
tf30-084	0.1126	0.6400	0.2100 %
tf30-085	0.1126	0.4200	0.1900 %
tf30-087	0.1126	0.5000	0.2200 %
tf30-088	0.1126	0.3800	0.2300 %
tf30-090	0.1126	0.3900	0.1700 %
tf30-091	0.1126	0.5900	0.1300 %
tf30-092	0.1126	0.3400	0.4800 %
tf30-094	0.1126	0.3000	0.2100 %
tf30-095	0.1126	0.2100	0.4300 %
tf30-096	0.1126	0.2100	0.4600 %
tf30-097	0.1126	0.2900	0.6300 %
tf30-098	0.1126	0.3700	0.3000 %
tf30-100	0.1126	0.2200	0.4300 %
tf30-102	0.1126	0.3500	0.1900 %
tf30-103	0.1126	0.2700	0.6000 %
tf30-105	0.1126	0.5000	0.1700 %
tf30-107	0.1126	0.3500	0.1700 %
tf30-109	0.1126	0.2500	0.4100 %
tf30-110	0.1126	0.2400	0.4200 %
tf30-111	0.1126	0.5700	0.1200 %
tf30-114	0.1126	0.5600	0.1000 %

Standards:	TCP	Water
tf30-002	2.6200 %	Unknown ppm
tf30-004	2.6900 %	1140.0000 ppm
tf30-005	2.6300 %	600.0000 ppm
tf30-006	2.7600 %	830.0000 ppm
tf30-007	2.7000 %	1190.0000 ppm
tf30-009	2.4800 %	1180.0000 ppm
tf30-010	2.4000 %	1150.0000 ppm
tf30-011	2.4200 %	830.0000 ppm
tf30-013	2.4200 %	850.0000 ppm

tf30-014	2.3700 %	1200.0000 ppm
tf30-015	2.3300 %	870.0000 ppm
tf30-018	2.3500 %	1410.0000 ppm
tf30-020	2.4000 %	800.0000 ppm
tf30-022	2.5200 %	730.0000 ppm
tf30-024	2.5400 %	1420.0000 ppm
tf30-025	2.4700 %	800.0000 ppm
tf30-026	2.6100 %	1510.0000 ppm
tf30-027	2.4500 %	1070.0000 ppm
tf30-028	2.5300 %	Unknown ppm
tf30-029	2.4400 %	1070.0000 ppm
tf30-031	2.5400 %	960.0000 ppm
tf30-032	2.6200 %	Unknown ppm
tf30-033	2.5600 %	890.0000 ppm
tf30-034	2.5700 %	620.0000 ppm
tf30-036	2.3700 %	1330.0000 ppm
tf30-037	2.3100 %	1270.0000 ppm
tf30-040	2.3600 %	1310.0000 ppm
tf30-041	2.3600 %	1260.0000 ppm
tf30-043	2.4300 %	900.0000 ppm
tf30-045	2.5600 %	880.0000 ppm
tf30-047	2.6400 %	1420.0000 ppm
tf30-048	2.7000 %	1350.0000 ppm
tf30-049	2.3200 %	1360.0000 ppm
tf30-050	2.2200 %	1490.0000 ppm
tf30-052	2.3200 %	1370.0000 ppm
tf30-053	2.3300 %	590.0000 ppm
tf30-054	2.2600 %	770.0000 ppm
tf30-055	2.3600 %	1370.0000 ppm
tf30-056	2.3100 %	Unknown ppm
tf30-057	2.3300 %	780.0000 ppm
tf30-058	2.4700 %	Unknown ppm
tf30-060	2.4300 %	790.0000 ppm
tf30-061	2.4600 %	Unknown ppm
tf30-063	2.5600 %	820.0000 ppm
tf30-067	2.5000 %	1120.0000 ppm
tf30-068	2.3700 %	780.0000 ppm
tf30-069	2.4400 %	610.0000 ppm
tf30-070	2.2800 %	630.0000 ppm
tf30-071	2.6000 %	610.0000 ppm
tf30-072	2.5900 %	790.0000 ppm
tf30-074	2.5700 %	760.0000 ppm
tf30-075	2.6000 %	670.0000 ppm
tf30-076	2.3600 %	800.0000 ppm
tf30-077	2.4900 %	570.0000 ppm

tf30-081	2.2400 %	570.0000 ppm
tf30-082	2.2600 %	800.0000 ppm
tf30-083	2.4500 %	520.0000 ppm
tf30-084	2.3900 %	1250.0000 ppm
tf30-085	2.5000 %	590.0000 ppm
tf30-087	2.6300 %	600.0000 ppm
tf30-088	2.4900 %	580.0000 ppm
tf30-090	2.6000 %	550.0000 ppm
tf30-091	2.3400 %	810.0000 ppm
tf30-092	2.4000 %	1210.0000 ppm
tf30-094	2.3700 %	700.0000 ppm
tf30-095	2.3300 %	1300.0000 ppm
tf30-096	2.3300 %	410.0000 ppm
tf30-097	2.5900 %	1420.0000 ppm
tf30-098	2.4000 %	1210.0000 ppm
tf30-100	2.3700 %	730.0000 ppm
tf30-102	2.4900 %	580.0000 ppm
tf30-103	2.5400 %	1260.0000 ppm
tf30-105	2.4200 %	490.0000 ppm
tf30-107	2.4900 %	460.0000 ppm
tf30-109	2.6200 %	500.0000 ppm
tf30-110	2.5300 %	410.0000 ppm
tf30-111	2.2900 %	420.0000 ppm
tf30-114	2.3400 %	680.0000 ppm

C.3. Model for Fuel Dilution

Method Summary: tf30fd

Method:

Name: tf30fd

Ident: PE IR SubTech Method BINARY QUANT+ 4.00

Version: 1

ID: 3036

Analyst: gam

Title:

Description: Analysis of Fuel Dilution in Mobil Jet Oil II from TF30 engines

Created: 05/12/2000 16:40:27

Last modified: 08/17/2000 12:27:33

Secured: No

No. of properties: 1

No. of standards: 21

Calibrated: No

Calculation Parameters:

Algorithm: PLS2
 Range: 4000 to 500 cm⁻¹
 Interval: 1 cm⁻¹
 Analysis Type: Absorbance
 Scaling (Spectra): Mean
 Scaling (Property): Unknown
 Smooth: Yes
 Smooth width: 19
 Baseline correction: Derivative
 Order: 2
 Width: 9
 Normalization: Norm. Factor
 Ordinate threshold:
 Upper threshold: 1.5 A
 Lower threshold: None
 Number of factors:
 Minimum: 1
 Maximum: 100
 Blank regions: 3010.00 to 2820.00 1790.00 to 1690.00 cm⁻¹
 1495.00 to 930.00 cm⁻¹

Property Values:

Standards:	Norm. Factor	FuelDilution
jetoil_0	0.1132	0.0000 %
jetoil_1	0.1132	1.0000 %
jetoil_2	0.1132	2.0000 %
jetoil_5	0.1132	5.0000 %
tf030_0	0.1132	0.0000 %
tf030_2	0.1132	2.0000 %
tf030_5	0.1132	5.0000 %
tf038_0	0.1132	0.0000 %
tf038_1	0.1132	1.0000 %
tf038_2	0.1132	2.0000 %
tf038_5	0.1132	5.0000 %
tf051_0	0.1132	0.0000 %
tf051_1	0.1132	1.0000 %
tf051_5	0.1132	5.0000 %
tf059_0	0.1132	0.0000 %
tf059_1	0.1132	1.0000 %
tf059_2	0.1132	2.0000 %
tf106_0	0.1132	0.0000 %
tf106_1	0.1132	1.0000 %

<u>tf106_2</u>	0.1132	2.0000 %
<u>tf106_5</u>	0.1132	5.0000 %

Appendix D: Explanation of principle component analysis

Principle Component Analysis (PCA) involves rotating and transforming the original, n , axis, each representing a variable, into new axes. The transformation is performed so that the new axes lie along the directions of maximum variance of the data with the constraint that the axes are orthogonal (variables are uncorrelated). PCA finds linear combinations of variables with the largest variance, applying normalised coefficients to the variables used.

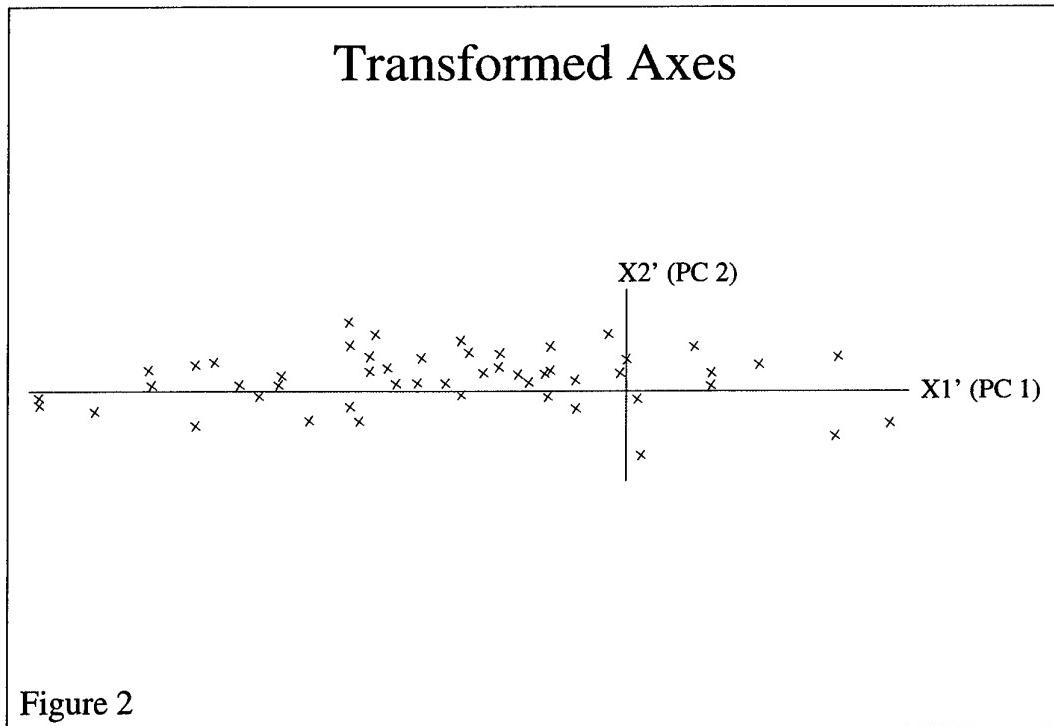
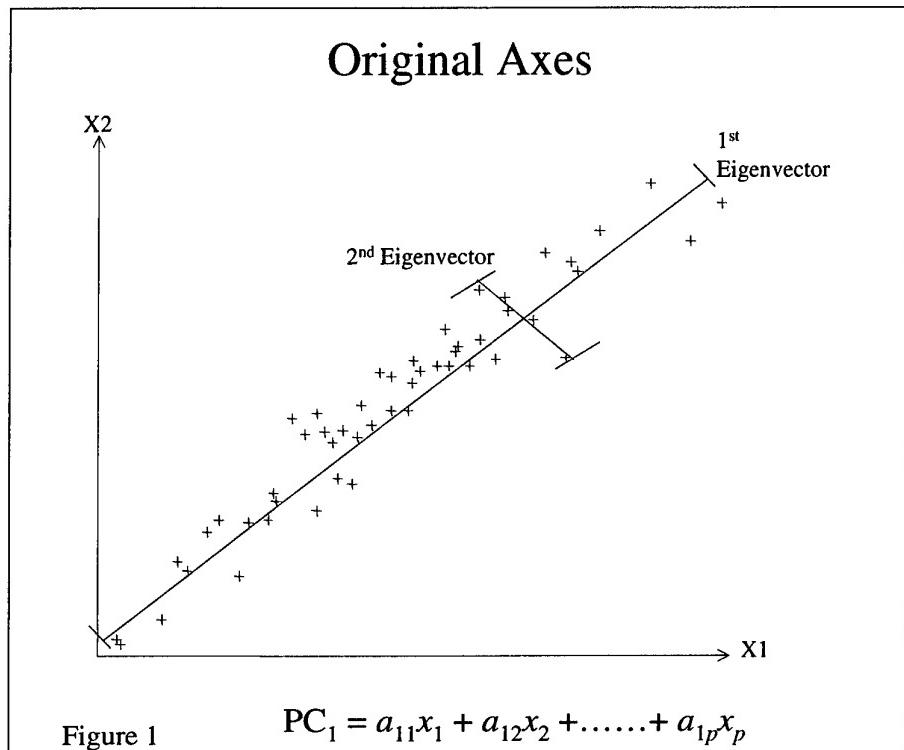
The first linear combination (or axis) is termed the first principal component (see equation on figure 1).

To visualise the process. Figure 1 represents a scatter plot of bivariate data. The first eigenvector, or principal component (PC), is drawn along the dimension of maximum variance. The second eigenvector (principal component) is drawn along the dimension of the next highest variance (as long as the principal components are orthogonal). If we had more than two variables, subsequent eigenvectors explain decreasing amounts of variance.

When the transformed axes are rotated (figure 2), the scores plot (original data projected onto transformed axes) can be used to reveal variables that contribute to the variance in the data.

If, for example, we wanted to know what variables were causing the spread of the data along PC1, we would inspect the loadings plots. The loadings are the coefficients of the eigenvectors, and the magnitude of the loading is indicative of the influence each variable has on a particular PC.

The length of the eigenvector is known as the eigenvalue, and the magnitude of the eigenvalue describes the amount of variance explained by that eigenvector. PCA is a useful technique because it reduces the dimensionality of the data and allows data to be visualised in fewer dimensions.



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Turbine Oils**

Paul Rawson and Geoff Morris

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<p>19. ABSTRACT To ensure optimum performance of military aircraft engines the chemical and physical condition of their oil must be monitored with time in service. Normal testing methods require a significant cost and time overhead. The ability for one test instrument to monitor the condition of the oil is an essential requirement of modern condition based oil analysis. This paper describes the use of a Fourier Transform Infrared (FTIR) instrument, coupled with the powerful chemometrics based analysis technique to monitor oil acidity, viscosity, load carrying additive, water and antioxidant concentrations from synthetic turbine oils from a series of in-service TF30 engines. The FTIR-Chemometrics based technique was found to offer confidant prediction of these oil condition properties and was found to be a suitable technique for oil condition monitoring for the TF30 engine oil system. Further refinement of the technique would be required before introduction into service for use by non-skilled operators.</p>			